NEW YORK UNIVERSITY WASHINGTON SQUARE COLLEGE OF ARTS AND SCIENCES MATHEMATICS RESEARCH GROUP

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A SELF CONSISTENT CALCULATION OF THE DISSOCIATION OF OXYGEN IN THE UPPER ATMOSPHERE

by
HARRY E. MOSES

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Project Director

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I. Introduction

The constituents of the upper atmosphere undergo dissociation and ionization under the influence of the intense solar radiation available at high altitudes. These processes are of interest because they are responsible for the layers of free electrons in the upper atmosphere which are so important in radio wave propagation. They are also of interest because they are responsible for the conversion of radiant energy into heat.

The processes in the upper atmosphere are so little understood that it appears impossible to treat the dissociation phenomena with complete generality. However, it seems possible to set up models for some of the processes which are useful in gaining insight into the nature of the phenomena. A process which appears amenable to theoretical treatment is the dissociation of oxygen in the upper atmosphere. This process is comparatively simple, and one can set up reasonable models which have internal consistency and can be used as a basis for making numerical calculations.

In a previous paper [1] a self-consistent model for the dissociation of oxygen was set up. The object of the present paper is to set up another model and to present numerical calculations based on it. Inasmuch as the model of the present paper has many features in common with that of reference 1, we shall review the assumptions upon which the model of reference 1 is based and indicate the modification which is made in the present paper. One of the more controversial assumptions will be dropped and another substituted.

1. The principal dissociation process is

$$O_2(x^3 \sum_g) + hv \xrightarrow{\sigma_y} O(^3p) + O(^1p)$$
 (1)

where hv is the energy of the quantum of radiation absorbed from the sunlight.

2. The principal recombination processes are two-body recombination processes in which two oxygen atoms recombine to form an oxygen molecule, the excess energy being in the form of radiation. A typical process of this sort is

$$O(^{3}P) + O(^{3}P) \xrightarrow{\beta_{D}^{\prime}} O_{2}(b^{1}\sum_{g}^{+}) + hv_{1} \longrightarrow O_{2}(x^{3}\sum_{g}^{-}) + hv$$
 (2)

where β'_n denotes the recombination cross section.

- 3. Dissociative equilibrium exists, so the rate of dissociation equals the rate of recombination at any altitude.
- 4. The rate of energy absorbed in process (1) equals the rate of emission of energy in process (2). This is the assumption which will be changed.
- 5. The time required to establish dissociative equilibrium is less than that required to establish diffusive equilibrium between the oxygen atoms and molecules.
- 6. There is diffusive equilibrium between the nitrogen and oxygen of the atmosphere.

There are, in addition, various assumptions of a less fundamental and a less controversial nature. They were used in reference 1 and will be brought up again in the present paper.

with the above assumptions it was shown to be possible to set up a system of three equations from which one can solve for the three fundamental unknowns: the temperature T, the number density of oxygen atoms n, and the number density of oxygen molecules n, all as functions of altitude x, provided certain boundary conditions were given. These boundary conditions were taken as the temperature and temperature gradient at some altitude x, within the region where dissociation takes place. The most striking feature of the resulting calculation was that the dissociation region was quite large, in contrast to the results of previous workers, who found that the region was quite narrow (see references 2-7).

It was emphasized in reference 1 that the numerical results must not be taken too seriously because it is not known how valid the assumptions 1-6 are, nor how accurately the cross sections \mathcal{G}_v and β_v' represented the experimental results. In particular β_v' had to be assumed, since no theoretical or experimental work had been done to determine this cross section. The principal result of reference 1 was to show that a self-consistent method could be set up with the assumptions 1-6, and hence that if in the future assumptions 1-6 can be shown valid and better values of the cross sections are available, the method indicated in reference 1 can be used. It should be noted that the assumptions made were self-consistent; it was not necessary to assume a distribution n_2 , which is one of the quantities to be calculated. It was shown that the work of some of the previous workers was not self-consistent in this sense n_2 .

^{1.} Appendix 7, Ref. 1

VI. Other Dissociation Models

Comparison of our present results with those of reference 1 show considerable differences. First of all, in reference 1 the region of dissociation is at the altitude for which $n_2 = 10^{12}$. Secondly, the dissociation is much broader, of the order 15 km. Thirdly, N_2 is much larger than the value obtained using the ordinary barometric equation, whereas in the present case it is smaller. The principal reasons for these differences are that we have dropped the energy balance requirement, assumption 4, and perhaps more important, that we have used different boundary conditions. In the present paper we have required explicitly that $N_2(x) \rightarrow 0$ as $x \rightarrow \infty$. In reference 1 we could not apply this condition explicitly because the theory of that paper was not valid at very high altitudes since the energy balance condition could not be satisfied there. It was necessary in the theory of reference 1 to assume that processes occurred such that $n_2(x)$ did not decrease too rapidly at high altitudes, but the discussion of such processes were outside the theory.

The results of the present model are more satisfactory than those of reference 1 in that $N_2(x) \rightarrow 0$ for $x \rightarrow \infty$ as required. However, this does not necessarily mean that the model of reference 1 is incorrect (although the numerical results seem untenable), since with more accurate cross sections the model of reference 1 might give results closer to those obtained in the present work, and, specifically, might lead to smaller values of N_2 .

An alternative way of trying to modify the model of reference 1 is the following:

If in the model of reference 1 one had taken as boundary conditions $N(x) \rightarrow 0$ as $x \rightarrow \infty$ and had given a value of n_2 at some altitude x_0 , one would have found that the temperatures calculated from the model would be of the order of a thousand degrees. This result suggests that in order to obtain more reasonable temperatures one should, in formulating the energy balance equations, take into account possible ways of conserving energy other than by the radiation processes (1) and (2); in particular, one should include heat conduction.

The present calculations indicate that the dissociation region occurs where the atmospheric density is so great that it is conceivable that three-body collisions are important as a recombination process. It is possible within the framework of the present paper to assume three-body recombinations rather than two-body recombinations.

Acknowledgments

The problem investigated in this paper is part of a program formulated under the direction of Mr. N. C. Gerson of the Ionospheric Laboratory, Geophysics Research Division, Air Force Cambridge Research Center. The author also wishes to acknowledge helpful discussions with Dr. Ta-You Wu.

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ABSTRACT

In a previous paper (ref. 1) a self-consistent model was set up for the dissociation of oxygen in the upper atmosphere under the assumption of mumber balance and radiative energy balance and a form of the barometric equation. In the present paper a similar model is used, but the requirement of radiative energy balance is dropped and a temperature distribution is assumed. The resulting calculations indicate that for this model the dissociation region is much narrower than in the previous model and that it occurs at lower altitudes.



I. Introduction

The constituents of the upper atmosphere undergo dissociation and ionization under the influence of the intense solar radiation available at high altitudes. These processes are of interest because they are responsible for the layers of free electrons in the upper atmosphere which are so important in radio wave propagation. They are also of interest because they are responsible for the conversion of radiant energy into heat.

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In a previous paper[1] a self-consistent model for the dissociation of oxygen was set up. The object of the present paper is to set up another model and to present mmerical calculations based on it. Inasmuch as the model of the present paper has many features in common with that of reference 1, we shall review the assumptions upon which the model of reference 1 is based and indicate the modification which is made in the present paper. One of the more controversial assumptions will be dropped and another substituted.

1. The principal dissociation process is

$$0_2(x^3 \sum_{g}^{-1}) + hv \rightarrow 0 (^3p) + 0(^3p)$$
 (1)

where hy is the energy of the quantum of radiation absorbed from the sunlight.

2. The principal recombination processes are two-body recombination processes in which two oxygen atoms recombine to form an oxygen molecule, the excess energy being in the form of radiation. A typical process of this sort is

$$O(^{3}\mathbf{P}) + O(^{3}\mathbf{P}) \xrightarrow{\beta'} O_{2}(\mathbf{b}^{1} \sum_{g}^{+}) + hv_{1} \longrightarrow O_{2}(\mathbf{x}^{3} \sum_{g}^{-}) + hv \qquad (2)$$

where $\beta_{\mathbf{v}}^{\prime}$ denotes the recombination cross section.

- 3. Dissociative equilibrium exists, so the rate of dissociation equals the rate of recombination at any altitude.
- 4. The rate of energy absorbed in process (1) equals the rate of emission of energy in process (2). This is the assumption which will be changed.
- 5. The time required to establish dissociative equilibrium is less than that required to establish diffusive equilibrium between the oxygen atoms and molecules.
- 6. There is diffusive equilibrium between the nitrogen and oxygen of the atmosphere.

There are, in addition, various assumptions of a less fundamental and a less controversial nature. They were used in reference 1 and will be brought up again in the present paper.

With the above assumptions it was shown to be possible to set up a system of three equations from which one can solve for the three fundamental unknowns: the temperature T, the number density of oxygen atoms n_p , and the number density of oxygen molecules n_2 , all as functions of altitude x, provided certain boundary conditions were given. These boundary conditions were taken as the temperature and temperature gradient at some altitude x_0 within the region where dissociation takes place. The most striking feature of the resulting calculation was that the dissociation region was quite large in contrast to the results of previous workers who found that the region was quite narrow (see references 2-7).

It was emphasized in reference 1 that the mumerical results must not be taken too seriously because it is not known how valid the assumptions 1-6 are, nor how accurately the cross sections $C_{\mathbf{v}}$ and $\beta_{\mathbf{v}}'$ represented the experimental results. In particular $\beta_{\mathbf{v}}'$ had to be assumed, since no theoretical or experimental work had been done to determine this cross section. The principal result of reference 1 was to show that a self-consistent method could be set up with the assumptions 1-6, and hence that if the future assumptions 1-6 can be shown valid and better values of the cross sections are available, the method indicated in reference 1 can be used. It should be noted that the assumptions made were self-consistent: it was not necessary to assume a distribution n_2 , which is one of the quantities to be calculated. It was shown that the work of some of the previous workers was not self-consistent in this sense n_1 .

^{1.} Appendix 7, Ref. 1

As indicated above, perhaps the most contreversial assumption is assumption 4, that of energy conservation through a radiative steady state. This assumption is questionable because energy processes other than (1) or (2) may occur, e.g. heat conduction. In this present paper we shall try to eliminate assumption 4. It will now no longer be possible to calculate all three quantities T, n₂, n_p as functions of altitude, as was done in reference 1, for we shall have too few equations. Instead we shall take the temperature T as given, and calculate n₂ and n_p as functions of the altitude under appropriate boundary conditions.

Dropping assumption 4, while having the disadvantage of compelling us to assume a value for T, has the advantage of making the resulting theory applicable over a larger range of altitudes. This is because assumption 4 can be true only in regions where processes (1) and (2) are principal processes leading to conversion of radiation to heat, whereas the treatment of the present paper will be true at any altitude, provided the atmospheric density is sufficiently low to permit one to assume two-body recombinations. As a result, we shall be able to impose boundary conditions on our equations at extremely high altitudes.

It is to be emphasized that in this paper, as in reference 1, the numerical calculations should not be taken too seriously. The numerical calculations are undertaken essentially to show the nature of the solution of the problem.

II. The Basic Equations

We shall now write the basic equations in some generality and later include our assumptions. The first of these equations is the number balance equation in which the number of dissociations per unit volume per second equals the number of recombinations per second. Let us consider the dissociation processes. It is generally agreed that the principal dissociation process is process (1) in which the oxygen molecule is dissociated from the normal electronic bound state to the dissociated state in the Runge-Schumann continuum on the absorption of radiation with a wave length smaller than 1750A. The cross section for this process has been studied experimentally in references 8 and 9

^{2.} See concluding paragraph of present paper.

and theoretically in reference 10. Denoting this cross section by σ_v as above, we have the number of dissociations per second at any altitude x given by

$$n_2(x) \int_{v}^{\infty} \frac{c}{hv} \, \sigma_v \, \rho_v(x) \, dv$$

where $\rho_{v}(x)$ is the radiation density per unit frequency available at the altitude x, $n_{2}(x)$ is the number density of oxygen molecules at the altitude x, and v_{0} is the threshold frequency corresponding to the wave length 1750A. Now, since there is attenuation of light by the oxygen molecules above the altitude x, we have

$$\rho_{v}(x) = \rho_{v}(\infty) e^{-\sigma_{v} N_{2}(x)}$$

$$N_{2}(x) = \int_{x}^{\infty} n_{2}(x) dx$$
(3)

where $\rho_v(\infty)$ represents the radiation density available at the "top" of the atmosphere. Then one can write

no. dissociations/sec =
$$n_2(x) I(N_2)$$
 (4)

$$I(\mathbf{N}_2) = \int \frac{\mathbf{c}}{hv} \, \sigma_v \, \rho_v(\infty) \, \bullet^{-\sigma_v N_2} \, \mathrm{d}v \, . \tag{5}$$

The number of recombinations per unit volume per second can be written as $n_p^2(x)$ B'(T) where $n_p(x)$ is the number density of oxygen atoms at altitude x and B'(T) is the recombination coefficient, which depends on the specific recombination assumed, and T is the temperature at the altitude x. The recombination coefficient depends upon the temperature because it has been averaged over the relative velocities of the atoms using the Boltzmann distribution characterized by a temperature T. Hence the equation of number balance is

$$n_2(x) I(N_2(x)) = n_p^2 B^{\dagger}(T).$$
 (6)

The barometric equation is

$$\frac{dP}{dx} = -g \left(Nn_p + 2Nn_2 + N_n n_n \right)$$

where P is the pressure at altitude x, g is the gravitational constant, M is the mass of the oxygen atom, $n_{\widetilde{N}}$ is the number density of nitrogen molecules, and M $_{\widetilde{N}}$ is the mass of the nitrogen molecule,

But
$$P = (n_{R} + n_{2} + n_{M}) kT$$
. (7)

Hence the barometric equation is

$$\frac{d}{dx} \left[(n_{\mathbf{p}} + n_2 + n_{\mathbf{N}}) \, kT \right] = - (Mn_{\mathbf{p}} + 2Mn_2 + M_{\mathbf{N}}n_{\mathbf{N}}) \, g, \tag{g}$$

Equations (6) and (8) are the basic equations of our theory. It should be noted that these equations are quite general and are largely independent of the model. In these equations we shall assume T and $n_{\rm H}$ as given functions of x. The unknown functions which we wish to solve for are $n_{\rm D}$ and $n_{\rm Z}$.

III. Detailed Model

We shall work with a model in which the radiation from the sun is equivalent to radiation from a black body of temperature 6000° K. Tegether with certain geometrical considerations, (see ref. 1) this assumption specifies $P_p(\infty)$. A more controversial assumption is that which determines $n_{\overline{n}}$ as a function of the altitude x. Most of the previous workers assume that the ratio of nitrogen to oxygen $\frac{n_{\overline{n}}}{n_2 + 2n_{\overline{p}}}$ has a constant value, namely 4, the

value of the ratio at the surface of the earth. This assumption requires that winds of sufficient frequency and strength occur so as to disturb diffusive equilibrium. If such winds occurred they would most likely also disturb the distribution of exygen atoms and molecules so that the problem of finding the dissociation ratio would be meaningless. We therefore take the alternative point of view, namely that diffusive equilibrium predominates between oxygen and nitrogen (assumption 6). This assumption means that oxygen

and nitrogen are distributed independently of each other. With this assumption we have

$$\frac{d}{dx} \left[\mathbf{n}_{\mathbf{N}} \, \mathbf{k} \, \mathbf{\bar{T}} \right] = - \, \mathbf{M}_{\mathbf{N}} \, \mathbf{n}_{\mathbf{N}} \, \mathbf{g} \tag{9}$$

and equation (8) becomes

$$\frac{d}{dx} \left[(n_p + n_2) kT \right] = - \left[Mn_p + 2Mn_2 \right] g$$
 (8a)

and all reference to the distribution of nitrogen in the barometric equation (8a) disappears.

The most controversial of the present assumptions is that which deals with the recombination process. Some of the previous workers (ref. 3,4,7) assume that recombination of the two oxygen atoms is given to a third body when the three bodies collide. Schematically

$$0 + 0 + M \longrightarrow 0_{2} + M^{*} \tag{10}$$

where M is the third body and the asterisk represents the third body in a wtate which is excited either internally or in the sense that it has greater translational energy.

Others (ref. 5,6) prefer to think of the recombination as being a twobody radiative process in which the excess energy is emitted in the form of radiation.

$$0 + 0 \longrightarrow 0_2 + hv. \tag{11}$$

For simplicity and in order to minimize the difference between the model of our present paper and that of reference 1 we assume two-body recombinations in the present calculation.

If one assumes a two-body process, it can be shown (ref. 1) that this process goes so slowly that virtually all the exygen atoms in the state ¹D, which is the result of the dissociation (equation (1)), will have had time to drop to the ³P state by emission of the forbidden red line

$$O(^{1}D) \rightarrow O(^{3}P) + hv_{red}$$
 (12)

so that virtually all the atoms are in the 3P state; hence the notation n for the atomic number density. Then the most probable recombination process, assuming two-body recombinations, is one typified by the equation

$$0(^{3}P) + 0(^{3}P) (^{1}\pi_{u}) \longrightarrow 0_{2}(b^{1}\sum_{g}^{+}) + hv$$
, (13)

and the rate of recombination is

$$n_{p}^{2} \int_{v=0}^{\infty} v \beta'_{v} f_{T}(v) dv ,$$

where v is the relative velocity of the two atoms, β' is the recombination cross section of process (13) and $f_{T}(v)$ is the Boltzmann distribution with respect to relative velocity v. Unfortunately the cross section $oldsymbol{eta}_{\mathtt{v}}'$ for process (13) is not known, but one can estimate it by assuming that within a statistical weight factor and a factor arising from a different threshold frequency it is much the same as the known cross section β_{ψ} for the process inverse to process (2), namely

$$O(^{3}P) + O(^{1}D) \longrightarrow O(x^{3} \sum_{g}) + hv. \qquad (2a)$$

Hence we can evaluate $B'(T) = \int_{-\infty}^{\infty} v \rho'_{T} f_{T}(v) dv$ of equation (6).

To replace assumption (4) we assume instead that $T = T_A + \propto (x-x_A)$ being the temperature of the altitude $x = x_0$ and ∞ being the gradient of the temperature. In point of fact it is sufficient to take $T = T_0 = const.$, because it turns out that the mamerical results are independent of \propto if \propto is sufficiently small ($\propto < 10^{\circ}/\mathrm{Km}$, say). This point will later be discussed more fully. However, we shall take arbitrary, since the equations are not essentially more complicated for this case.

IV. The Basic Equations and the Method of Solution

The basic equations for the calculations are the number balance equation

$$I(N_2)n_2 = B'(T)n_p^2 \tag{6}$$

 $I(N_2)n_2 = B'(T)n_p^2$ and the barometric equation which for $T = T_0 + \alpha(x-x_0)$ has the following form:

$$\frac{d(n_2 + n_p)}{dx} = -\frac{1}{T} \left\{ \alpha (n_2 + n_p) + \frac{Mg}{k} (n_p + 2n_2) \right\},$$
 (gb)

 $I(N_2)$ and B'(T) have been calculated and are given graphically as functions of their arguments in figures 1 and 2.

To solve the equations (6) and (9b) it is convenient to introduce the total number density

$$f(x) = n_2(x) + n_1(x).$$
 (14)

From (14) and (6) one obtains

$$n_2 = \left(\frac{-\sqrt{\frac{I(N_2)}{B(T)}} + \sqrt{\frac{I(N_2)}{B(T)}} + \mu_f}{2}\right)$$
(15)

$$n_{p} = \frac{-1 + \sqrt{1 + \frac{B(T)}{I(N_{2})}}}{2 \frac{B(T)}{I(N_{2})}},$$
(16)

and (8b) can be written either as

$$\frac{\mathrm{d}\mathbf{f}(\mathbf{x})}{\mathrm{d}\mathbf{x}} = -\frac{1}{T} \left\{ \left(\frac{\mathrm{Mg}}{k} + \propto \right) \ \mathbf{f}(\mathbf{x}) + \frac{\mathrm{Mg}}{k} \ \mathbf{n}_{2}(\mathbf{x}) \right\}$$
 (17)

or

$$\frac{\mathrm{d}\mathbf{f}(\mathbf{x})}{\mathrm{d}\mathbf{x}} = -\frac{1}{\mathrm{T}} \left\{ \left(\frac{2Mg}{k} + \alpha \right) \mathbf{f}(\mathbf{x}) - \frac{Mg}{k} \mathbf{n}_{\mathbf{p}}(\mathbf{x}) \right\}. \tag{18}$$

It is convenient to consider (17) and (15) as the differential equation for f(x) when $n_2(x)$ is small and (18) and (16) as the differential equation for f(x) when $n_p(x)$ is small, though both sets of equations are, of course, the same. Of course we use $\int_{x}^{\infty} n_2(x) = N_2$ in either case.

At high altitudes where n_2 is very small compared to n_p , it is seen that $f(x) = n_p$ and that equation (17) is the ordinary barometric equation for n_p . The density $n_2(x)$ is given by (15) which, since f(x) is small too (but much larger than $n_2(x)$), becomes

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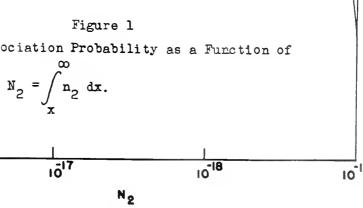
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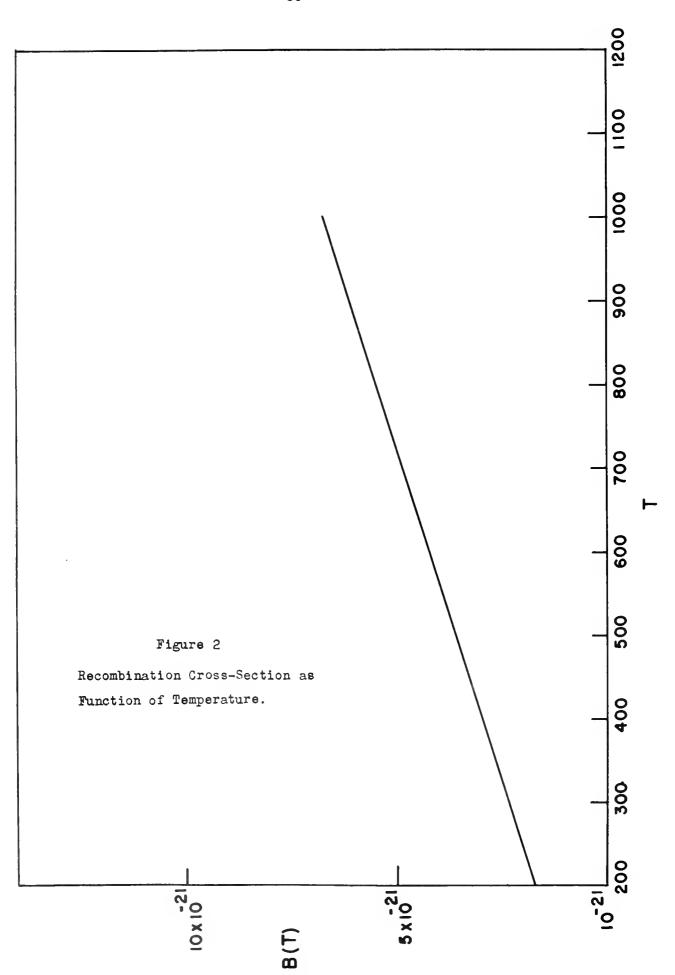
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I(N⁵)





$$n_2(x) = \sqrt{\frac{I(H_2)}{B(T)}} f(x) = \sqrt{\frac{I(H_2)}{B(T)}} n_p$$
, (19)

which is just equation (6). Thus for high altitudes, the oxygen atoms behave just like an ordinary gas without dissociation present, and n_2 is given by equation (6).

For high altitudes where $N_2 \rightarrow 0$ so that $I(N_2) \rightarrow I(0) = \text{const.}$, and for the case that T is a constant at these altitudes, $n_2(x)$ also satisfies the ordinary barometric equation as is clear from (19).

For low altitudes where N_2 is large and n_p small, $f(x) = n_2(x)$ to a very good approximation and equation (18) becomes the ordinary barometric equation for $n_2(x)$. That is if $n_2(x)$ were prescribed at x_0 for x_0 sufficiently low, both the barometric equation with and without dissociation would give the same result for $n_2(x)$ at low altitudes. $n_p(x)$ is given by (17) which becomes

(since
$$\frac{f(x)}{I(N_2)}$$
 is large)
$$n_p = \sqrt{\frac{B(T)}{I(N_2)}} = \sqrt{\frac{B(T)n_2(x)}{I(N_2)}}$$
(20)

which is just equation (6).

Thus for low altitudes $n_2(x)$ obeys the ordinary barometric equation whereas for high altitudes $n_p(x)$ obeys it; in the intermediate region neither does, and $n_p(x)$ and $n_2(x)$ influence each other greatly with the consequence that $n_2(x)$ falls much more rapidly than predicted by the ordinary barometric equation.

Equations (17) and (15) or, equivalently, (18) and (16) were solved by the following scheme:

One prescribes $n_2(x_0)$ and takes for $N_2(x_0)$ the result predicted by the ordinary barometric equation, just to have some starting value for $N_2(x_0)$.

Using equation (6) for $x = x_0$, $n_p(x_0)$ can be found, and from (14) one obtains $f(x_0)$. Then using (17) one can solve for f(x) by a step-by-step integration. For example, for $x_1 = x_0 + \Delta_1 x$ one has

$$f(x_1) = f(x_0) + \frac{df}{dx} \Big|_{x=x_0} \triangle_1 x$$

where
$$\frac{df}{dx}\Big|_{x=x_0}$$
 is computed from (17).

One then has

$$N_2(x_1) = N_2(x_0) - n_2(x_0) \triangle_1 x$$

and can compute $n_2(x_1)$ from (15), since $f(x_1)$ and $I(B_2)$ at $x = x_1$ are now known.

Further,
$$n_p(x_1) = f(x_1) - n_2(x_1)$$
 and $\frac{df}{dx} \Big|_{x=x_1}$ can be found from (18).

The procedure is repeated for $x_2 = x_1 + \Delta_2 x$ and one integrates to as high an altitude as one wishes.

One ultimately gets distributions $n_p(x)$, $n_2(x)$, $N_2(x)$ based on the choice of $N_2(x)$. The curve for $N_2(x)$ does not approach 0 as $x\to\infty$. Instead, one gets a curve which approaches a constant $N_{2\min}$

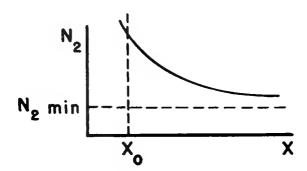
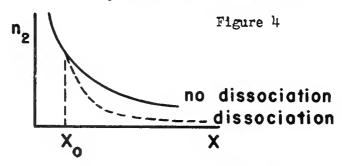


Figure 3

In order to get a better value of $N_2(x_0)$ one takes the old value of $N_2(x_0)$ and subtracts $N_{2\min}$. Using the new value of $N_2(x_0)$ one repeats the calculation. Again one finds a curve for $N_2(x)$ similar to the one above except that $N_{2\min}$ is much smaller (of course, one wishes it to be 0). One takes still a third value of $N_2(x_0)$ which consists of the second value of $N_2(x_0)$ minus the second value of $N_{2\min}$ and the integration is repeated. One eventually gets a value of $N_{2\min}$ which is so small and occurs at such a large value of x, that at and below the region at which dissociation becomes important the results are no

longer sensitive to N_{2min} . At this point the iteration procedure stops; 6 iterations were required in the calculations.

The final result is the following. At low altitudes the curves for $n_2(x)$ with and without dissociation agree if the curves are fitted at some point x_0^t (which may be less than x_0) where there is virtually no dissociation.



For low enough altitudes the curves for $N_2(x)$ with and without dissociation will also agree because in either case the most important contribution to $N_2(x)$ at low altitudes (well below x_0) comes from the value of $n_2(x)$ within a few kilometers of x. This is because $n_2(x)$ in both cases is relatively very small for x at any distance from the altitude being considered.

The important feature of the present treatment is that aside from assigning a boundary value n_2 at $x=x_0$, no a priori assumption is made on the distribution of $n_2(x)$ or equivalently on the function $N_2(x)$. These distributions are obtained from the basic equations. In all of the previous work on the oxygen dissociation problem (except in reference 1) such a priori assumptions are made, as pointed out in Appendix 7 of reference 1. For example, Penndorf (ref. 7) appears to assume that one may take $N_2(x)$ (equivalently $n_2(x)$) as though it were given by the ordinary barometric equation when no dissociation is present; i.e., he assumes dissociation has only a minor effect on the overall-distribution of n_2 . It will be seen below that this is not true, at least with the cross sections used.

V. Results of Numerical Calculations

Three cases were calculated numerically. In all three cases n_2 at $x=x_0$ was taken as $10^{14}/\text{cm}^3$. (If 0_2 is assumed to constitute 1/5 of the atmosphere, x_0 would correspond to 85 km.) This choice is not special though it may seem so since $n_2(x)$, $n_p(x)$ depend only on the difference $x-x_0$. The three different cases correspond to different choices of the temperature function $T = T_0 + x_0$. In the first case T_0 was taken as 195^0 and x_0 was taken as $5^0/\text{km}$. In the second case $T_0 = 200^0 \text{k}$, $x_0 = 0$.

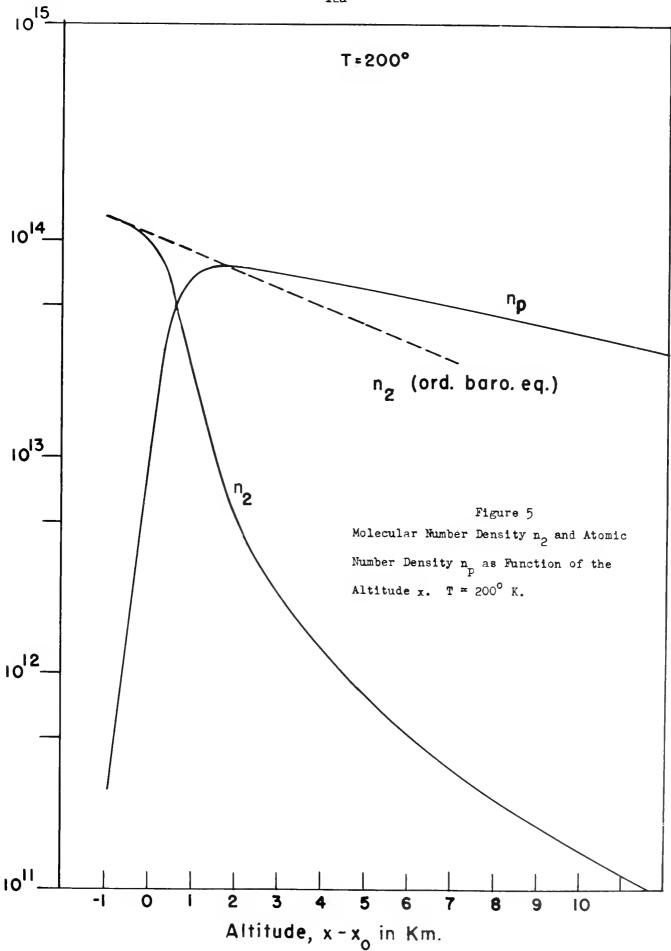
In the third case $T_0 = 300^{\circ} k$, $\approx = 0$. Comparison of results for the first and second cases gave essentially the same results, indicating that small temperature gradients do not affect the results greatly. This consequency is due to the smallness of the region in which dissociation is important; if the temperature has not too large a gradient in this small region, the temperature is essentially constant.

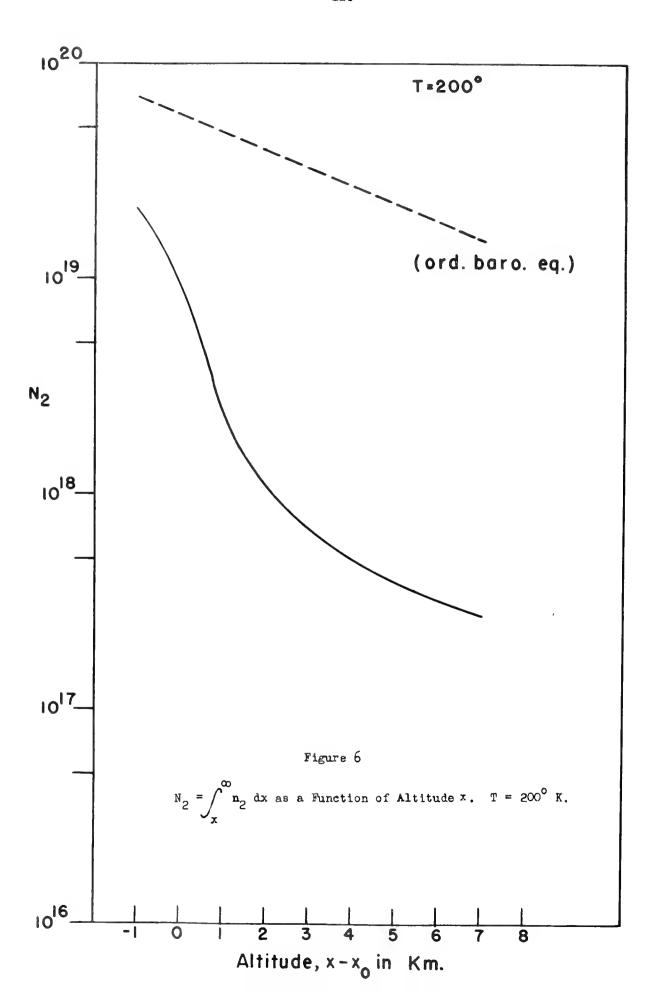
Since the first and second cases agree so closely, we have given graphs only of the second and third cases. Figures 5 and 6 represent the results for the second case, and figures 7 and 8 the results for the third case.

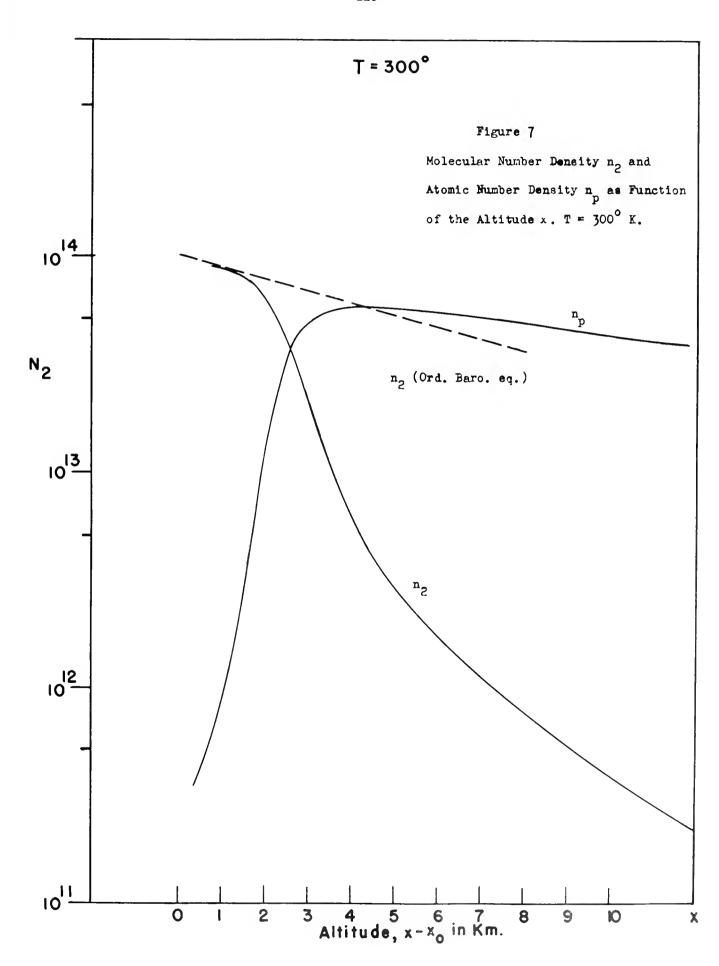
As is seen in both cases, the dissociation takes place in a very narrow region of the order of a kilometer near the altitude at which $n_2 = 10^{14}$, (hence the choice $n_2(x_0) = 10^{14}$). The effect of the higher temperature is to spread out the region of dissociation and raise the altitude of this region. N_2 is much larger for the higher temperature, the reason being that $n_2(x)$ decreases more slowly with the higher temperature.

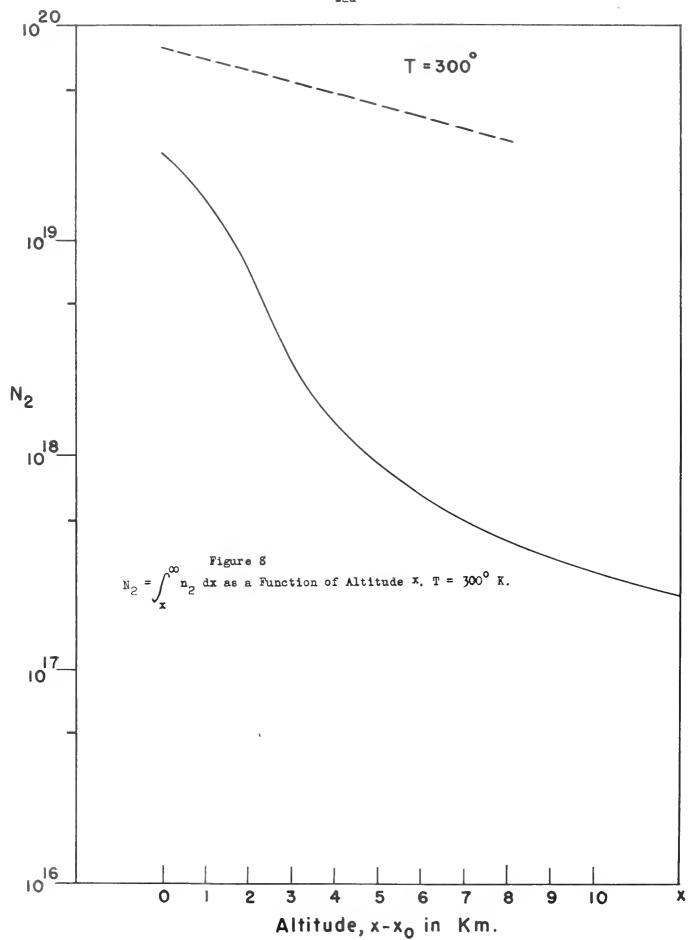
Also indicated on the graphs are the results when the ordinary baro-

metric equation without dissociation is used for $n_2, n_2 = n_{20}$ where n_{20}^1 and x_0^1 are chosen so that they coincide with the value obtained for $n_2(x)$ at sufficiently low altitudes. It is clear that in the region of dissociation and above that region, $n_2(x)$, $N_2(x)$ deviate considerably from the values obtained from the ordinary barometric equations. Hence the use of the ordinary barometric equations to give values of $n_2(x)$, $N_2(x)$ is incorrect.









VI. Other Dissociation Models

Comparison of our present results with those of reference 1 show considerable differences. First of all, in reference 1 the region of dissociation is at the altitude for which $n_2 = 10^{12}$. Secondly, the dissociation is much broader, of the order 15 km. Thirdly, N_2 is much larger than the value obtained using the ordinary barometric equation, whereas in the present case it is smaller. The principal reasons for these differences are that we have dropped the energy balance requirement, assumption 4, and perhaps more important, that we have used different boundary conditions. In the present paper we have required explicitly that $N_2(x) \rightarrow 0$ as $x \rightarrow \infty$. In reference 1 we could not apply this condition explicitly because the theory of that paper was not valid at very high altitudes since the energy balance condition could not be satisfied there. It was necessary in the theory of reference 1 to assume that processes occurred such that $n_2(x)$ did not decrease too rpaidly at high altitudes, but the discussion of such processes were outside the theory.

The results of the present model are more satisfactory than those of reference 1 in that $N_2(x) \longrightarrow 0$ for $x \longrightarrow \infty$ as required. However, this does not necessarily mean that the model of reference 1 is incorrect (although the numerical results seem untenable), since with more accurate cross sections the model of reference 1 might give results closer to those obtained in the present work, and, specifically, might lead to smaller values of N_2 .

An alternative way of trying to modify the model of reference l is the following:

If in the model of reference 1 one had taken as boundary conditions $N(x) \longrightarrow 0$ as $x \longrightarrow \infty$ and had given a value of n_2 at some altitude x_0 , one would have found that the temperatures calculated from the model would be of the order of a thousand degrees. This result suggests that in order to obtain more reasonable temperatures one should, in formulating the energy balance equations, take into account possible ways of conserving energy other than by the radiation processes (1) and (2); in particular, one should include heat conduction.

The present calculations indicate that the dissociation region occurs where the atmospheric density is so great that it is conceivable that three-body collisions are important as a recombination process. It is possible within the framework of the present paper, to assume three-body recombinations rather than two-body recombinations. Such a model would require more secondary assumptions such as the efficiencies of the various possible third bodies and their distribution. A calculation, similar to the present one but using the assumption of three-body recombinations, is being carried out and will be reported separately.

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